The Complex Analytic Structure of the Bands in Linear Molecular Chains

Emil Prodan

Center for Complex Materials, Princeton University, Princeton, NJ 08544, USA

In a classic paper [1], Walter Kohn found that the band energies of periodic Schroedinger operators in 1 dimension have a beautiful structure when one lets the k-wavevector be complex. He discovered that the energies of different bands are nothing but the same function evaluated on different sheets of a certain Riemann surface. This Riemann surface is generic in 1 dimension, in the sense that its shape does not depend on the particular form of the periodic potential. The asymptotic behavior of almost all correlation functions can be computed from the Riemann surface. In particular, properly defined Wannier functions decay exponentially with a decay rate dictated by the branch points of the Riemann surface.

In this talk I will review recent results [2] that generalize all the above to linear molecular chains in 3D. They are based on a new approach, which is quite different from the original one. The approach relies on topological arguments (plus elementary functional analysis) rather than the theory of second order differential equations. Based on this, I will discuss the generic structure of the Riemann surface for periodic molecular chains and present several explicitly computed examples.

I will conclude with a discussion of the exponential localization of the Wannier and Green's functions and of the density matrix. If time allows, I will also cover some recent applications to electronic nearsightedness [3] and transport [4].

[1] W. Kohn, Phys. Rev. **115**, 809 (1959).

[2] E. Prodan, Phys. Rev. B **73**, 035128 (2006).

[3] E. Prodan and W. Kohn, PNAS **102**, 11635 (2005).

[4] E. Prodan and R. Car, cond-mat/0702192 (2007).